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Commentary: The Hash House Harriers and the winding path to materials discovery

Abstract

Materials science research can be both very demanding and extremely rewarding. In this Commentary, in my own research of new electronic and magnetic materials, I give numerous exemplars of the path followed to materials discovery. I also highlight the parallels between my research experiences with the pastime of running. I hope that my thoughts will help guide junior researchers along the often tortuous and exciting path to new materials and that I can teach them to be open minded and persistent about following new lines of discovery. "No-pain, no-gain" applies to many things in life, running and scientific research being just two examples, but I hope in the case of scientific research that I can convince you the gain normally outweighs the pain.

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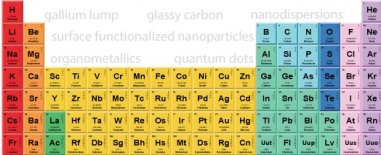
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Commentary: The Hash House Harriers and the winding path to materials discovery

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Materials science research can be both very demanding and extremely rewarding. In this Commentary, in my own research of new electronic and magnetic materials, I give numerous exemplars of the path followed to materials discovery. I also highlight the parallels between my research experiences with the pastime of running. I hope that my thoughts will help guide junior researchers along the often tortuous and exciting path to new materials and that I can teach them to be open minded and persistent about following new lines of discovery. “No-pain, no-gain” applies to many things in life, running and scientific research being just two examples, but I hope in the case of scientific research that I can convince you the gain normally outweighs the pain. © 2015 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License. [<http://dx.doi.org/10.1063/1.4917192>]

Over the past decades, my group has often ended up making samples or measurements that originally I never had any intention of ever doing because I considered them too finicky or esoteric. In each case, the physics or chemistry of the compound or ground state I was interested in ended up leading us to complex growth and physical property measurement extremes. We have measured de-Hass van-Alphen oscillations, studied vortex lattice phase transitions and spin-glass relaxation, pushed superconductivity to new extremes, studied field induced quantum criticality, grown single grain quasi-crystals, and mastered the use of Mg, Li, Zn, and As as components of high temperature solutions. I had always thought that these materials or measurements would require too low of a temperature, too high of a magnetic field, or simply be too difficult for us to work with, but such is life: the compounds we devised/developed made it clear that, in order to follow the physics, we need to go to these extremes. In this way, new materials remind me of a stubborn, unyielding, mule; you either follow them where they lead or give up on them and walk a different path. At other times, new materials remind me of the Hash House Harriers: they lead you where they want to and, although mildly painful, the trek is mostly well worth the effort.

Now, I must confess that I consider jogging to be a form of cosmic torture; I love to walk, but jogging...never.... Well, as Gilbert and Sullivan would say, “hardly ever.”¹ I stumbled upon the Hash House Harriers as an undergraduate at the University of Virginia, but I was told by a British collaborator that they originated “in the colonies” and, at this point in time, are popular throughout the world. The Harriers came up with a way of making jogging just a little more fun. On Friday afternoons, the hills around U.Va. (the hills of Jefferson’s dreams and secrets and the hills of Poe’s nightmares) would ring out with calls of “On-On, On-On!” These were the Harriers following the trail.

Each week one of the Harriers would create a trail by leaving flour marks on the roads and woodland paths over a wide swath of countryside. There were obfuscations, detours, and false trails.² The pack would then spread out and search for the marks, and when one was found, there would be a cry of “On-On.” The pack would move in an amoeba-like fashion over the countryside until it came to the end of the trail, where there would be a keg of beer and snacks. I guess this is the jogging equivalent of a fox hunt, although far better than Oscar Wilde’s “the unspeakable in full pursuit of the uneatable,”³ perhaps more like the fatigable chasing the drinkable.

When we come across a new material, it is like the start of a new run with the Harriers: we will have to search around to see what the physics of interest is and, when a measurement or an idea reveals

a promising trail, one of us will cry “On-On.” Sometimes it is a false trail, but sometimes it leads to new territory. Any new excursion has to have a starting point; in the case of the RTM_2Zn_{20} compounds (R = rare earth and TM = transition metal),^{4,5} I wanted to see what happened in well-ordered, large unit cell compounds, ideally with small amounts of rare earth and transition metal. In essence, I wanted to study dilute rare earth and dilute transition metal compounds. This starting point led to a compilation of crystal structures. NaCl or simple Cu structures would come first, but things then progressed in complexity and size of the unit cell. An entry that caught my eye was that of the RTM_2Zn_{20} materials, one unique R -site, one unique TM -site, and 3 Zn sites. If these compounds could be made in a controlled and clean fashion, then they could be queried in a variety of ways. So, at this point, the trial was laid and the chase began.

The first search and circling is to find out if we can grow the material. If that path can be found, then we need to see what sort of material the compound will be. In the case of the RTM_2Zn_{20} materials, we were able to grow large, faceted, jewels of single crystals (see Figure 1), but there was virtually no physical data other than unit cell parameters; we were in terra incognita. This is a time analogous to the Harrier pack circling and looking for the trail. We performed basic thermodynamic and transport measurements on various members of the family (R = Gd, Tb, Y, Lu and TM = Fe, Co, Ru, Rh) and found the lay of the land, letting the material start to whisper to us about what it has to offer. Suddenly, “On-On” came the call and we had a set of materials that could have local moments embedded in an electron sea that could be tuned to the edge of a Stoner instability.⁴ We then explored the rare earth series, a well-known path, until we hit the penultimate member, Yb. Then, the path again became muddy and confused until we made all six (TM = Fe, Co, Ru, Rh, Os, Ir) members of the $YbTM_2Zn_{20}$ family and realized that, as part of this trek, we have formally doubled the number of known Yb-based heavy fermions,⁵ thereby enabling us to study 4f and 3d correlations in a large, new family of closely related compounds.

For the Harriers, selecting the right shoes for a particular jog is a precondition for some treks. The RTM_2Zn_{20} compounds required that we address that high vapor pressure of Zn (over 1 atmosphere by 1000 °C). Based on the mastery of Zn as a solvent, we decided to, “see what we could do with Zn” and try to grow some completely different, binary, Zn compounds that had very low peritectic-decomposition temperatures. This was supposed to be “an easy trail” since I was taking some undergraduates out for their first trip around the periodic table. One morning we decanted⁶ a growth and suddenly the call of “On-On” rang like a clarion call throughout the lab. Under the microscope was a five-fold facet of a pentagonal dodecahedra. On what should have been a gentle path we came across a unicorn-like beast. Quite unintentionally, we had found a rare example of a

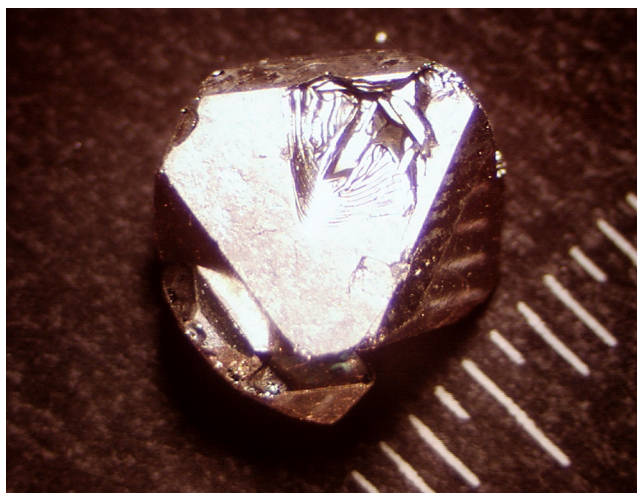


FIG. 1. A single crystal of RTM_2Zn_{20} grown out of excess Zn. These compounds actually seem eager to grow as large, well-formed crystals. Combine this with fascinating 4f- and 3d-shell physics and you have a huge new physical and compositional phase space to explore. Photo credit: S. Jia.

stable, binary quasicrystal (QC).⁷ As we understood the implication of this discovery, we proposed a possible route to finding other, undiscovered examples of binary QC systems (look for compounds near crystalline systems with quasicrystalline motifs in their unit cells that may have very low peritectic decomposition temperature).^{7,8} This proposal, of course, suggested another possible trail. Recently, we suited up, followed the markings, and indeed discovered an even rarer beast: a *R*-Cd based, local moment bearing family of binary quasicrystals.⁸ As we followed the trail, further spin-glass physics soon emerged.⁸

Another trail originated with the discovery in 2008 of FeAs-based superconductors.^{9,10} We wanted to determine the extent and properties of this new class of Fe-based superconductors.¹¹ As a part of this effort, we spread out over the country side and the group would call “On-On” as new paths and trails were revealed. One of these trails led to the discovery of a new compound: CaFe_2As_2 .¹² This compound was the logical end point of the BaFe_2As_2 , SrFe_2As_2 , and CaFe_2As_2 progressions up the alkali earth column, but it had not been discovered until we grew single crystals of it out of Sn solvent. What was not logical, or anticipated, was the degree to which CaFe_2As_2 had its moods and requirements. CaFe_2As_2 demanded to be handled with great care; it is exceptionally pressure and strain dependent.¹³ In order to understand this compound, we had to commit to detailed analyses of process–property relations^{14,15} as well as even pay attention to what type of grease we used to mount crystals for measurement. We found that CaFe_2As_2 is a wonderful system, it is an inorganic superconductor with organic-like sensitivities,¹⁶ it serves as a key example of FeAs-based superconductivity, but we had to be willing to pay the price and understand the trail we were jogging on.

I find myself thinking about the Harriers a lot these days. The past few years have been full of lovely jogs and trails and, with anticipation, I hope for several in the very near future, as well as many more after that. We have started to explore what can be grown out of reactive element fluxes. Li, Na, Mg, and Ca offer powerful solubility, very light masses, and the potential of incorporating other light, volatile, and refractory elements.¹⁷ (A remarkable surprise was the recent discovery of rare earth like magnetic anisotropies and molecular magnet like tunneling in Fe substituted Li_3N .¹⁸) Exploration of the transition metal rich corners of rare-earth-bearing ternary phase diagrams may lead to cheaper ferromagnets and the exploration of “fragile” antiferromagnets may lead to new high- T_c superconducting systems. This is the beauty and the allure of experimental condensed matter physics; there are many trails to follow not only false ones to identify but also true ones to pursue. The Harriers are just over the next hill and I hear the call of “On-On.” All I can do is try to follow.

Whereas what I have described above has group-specific idiosyncrasies, the broader outline of how new materials research is done is, I think, overarching across groups, academic departments, and nations. The discoveries of quasicrystals,¹⁹ $\text{Nd}_2\text{Fe}_{14}\text{B}$ ferromagnets,²⁰ superconductivity in MgB_2 ,²¹ and the $\text{RNi}_2\text{B}_2\text{C}$ quaternary superconductors,^{22,23} just to name a few systems, all came from such jogs through the mixed phase space of ideas and compositions. It is important to have ideas and efficient methods and tools for implementing and testing which ideas are good and which ones are not. Ultimately, making a materials and testing it is the most important step. As stated by Sophocles, “the unsought goes undetected.”

I would like thank U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering (Contract No. DE-AC02-07CH11358) for supporting and encouraging such jogs over the decades. In addition, I would like to thank the Gordon and Betty Moore Foundation EPIQS initiative (Grant No. GBMF4411) for helping a new group of joggers to suit up.

¹ W. S. Gilbert and A. Sullivan, *H.M.S. Pinafore* (A. S. Seer, New York, 1879).

² For a summary of the Hash House Harriers’ history and traditions please see http://en.wikipedia.org/wiki/Hash_House_Harriers.

³ O. Wilde, *A Woman of No Importance* (Methuen & Co. Ltd., 1894).

⁴ S. Jia, S. L. Bud’ko, G. D. Samolyuk, and P. C. Canfield, *Nat. Phys.* **3**, 334-338 (2007).

⁵ M. S. Torikachvili, S. Jia, E. D. Mun, S. T. Hannahs, R. C. Black, W. K. Neils, D. Martien, S. L. Bud’ko, and P. C. Canfield, *Proc. Natl. Acad. Sci. U. S. A.* **104**(24), 9960-9963 (2007).

⁶ P. C. Canfield and Z. Fisk, *Philos. Mag. Part B* **65**, 1117 (1992).

- ⁷ P. C. Canfield, M. L. Caudle, C.-S. Ho, A. Kreyssig, S. Nandi, M. G. Kim, X. Lin, A. Kracher, K. W. Dennis, R. W. McCallum, and A. I. Goldman, *Phys. Rev. B* **81**, 020201 (2010).
- ⁸ A. I. Goldman, T. Kong, A. Kreyssig, A. Jesche, M. Ramazanoglu, K. W. Dennis, L. Bud'ko, and P. C. Canfield, *Nat. Mater.* **12**, 714-718 (2013).
- ⁹ Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, *J. Am. Chem. Soc.* **130**, 3296 (2008).
- ¹⁰ M. Rotter, M. Tegel, and D. Johrendt, *Phys. Rev. Lett.* **101**, 107006 (2008).
- ¹¹ P. C. Canfield and S. L. Bud'ko, *Annu. Rev. Condens. Matter Phys.* **1**, 27-50 (2010).
- ¹² N. Ni, S. Nandi, A. Kreyssig, A. I. Goldman, E. D. Mun, S. L. Bud'ko, and P. C. Canfield, *Phys. Rev. B* **78**, 014523 (2008).
- ¹³ P. C. Canfield, S. L. Bud'ko, N. Ni, A. Kreyssig, A. I. Goldman, R. J. McQueeney, M. S. Torikachvili, D. N. Argyriou, G. Luke, and W. Yu, *Physica C* **469**, 404-412 (2009).
- ¹⁴ S. Ran, S. L. Bud'ko, D. K. Pratt, A. Kreyssig, M. G. Kim, M. J. Kramer, D. H. Ryan, W. N. Rowan-Weetaluktuk, Y. Furukawa, B. Roy, A. I. Goldman, and P. C. Canfield, *Phys. Rev. B* **83**, 144517 (2011).
- ¹⁵ S. Ran, S. L. Bud'ko, W. E. Straszheim, J. Soh, M. G. Kim, A. Kreyssig, A. I. Goldman, and P. C. Canfield, *Phys. Rev. B* **85**, 224528 (2012).
- ¹⁶ E. Gati, S. Köhler, D. Guterding, B. Wolf, S. Knöner, S. Ran, S. L. Bud'ko, P. C. Canfield, and M. Lang, *Phys. Rev. B* **86**, 220511 (2012).
- ¹⁷ A. Jesche and P. C. Canfield, *Philos. Mag.* **94**, 2372 (2014).
- ¹⁸ A. Jesche, R. W. McCallum, S. Thimmaiah, J. L. Jacobs, V. Taufour, A. Kreyssig, R. S. Houk, S. L. Bud'ko, and P. C. Canfield, *Nat. Commun.* **5**, 4333/1 (2014).
- ¹⁹ D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, *Phys. Rev. Lett.* **53**, 1951 (1984).
- ²⁰ J. J. Croat, J. F. Herbst, R. W. Lee, and F. E. Pinkerton, *J. Appl. Phys.* **55**, 2078 (1984).
- ²¹ J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani, and J. Akimitsu, *Nature* **410**, 63 (2001).
- ²² R. Nagarajan, C. Mazumdar, Z. Hossain, S. K. Dhar, K. V. Gopalakrishnan, L. C. Gupta, C. Godart, B. D. Padalia, and R. Vijayaraghavan, *Phys. Rev. Lett.* **72**, 274 (1994).
- ²³ R. J. Cava, H. Takagi, H. W. Zandbergen, J. J. Krajewski, W. F. Peck, Jr., T. Siegrist, B. Batlogg, R. B. van Dover, R. J. Felder, K. Mizuhashi, J. O. Lee, H. Eisaki, and S. Uchida, *Nature* **367**, 252 (1994).